time-dependent Schödinger equation

particle		wave
p	$=$	$\hbar k$
E	$=$	$\hbar\omega$

dispersion relation

photons $\omega = ck$

electrons $E = \dfrac{p^2}{2m}$

solution $e^{i(kz-\omega t)}$

$$\frac{1}{c^2}\frac{\partial^2\Phi}{\partial t^2} = \frac{\partial^2\Phi}{\partial z^2}$$

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial z^2}$$

time-dependent Schrödinger equation (TDSE)

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r},t)\right)\Psi(\vec{r},t)$$

1st derivative: initial-value problem for complex wave functions

$$\Psi(\vec{r},t+\Delta t) \approx \Psi(\vec{r},t) + \frac{\partial\Psi(\vec{r},t)}{\partial t}\Delta t$$

continuity equation for probability density

time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r},t)\right)\Psi(\vec{r},t)$$

Born interpretation:

$|\Psi(r,t)|^2$ is probability density for finding particle at time t at position r

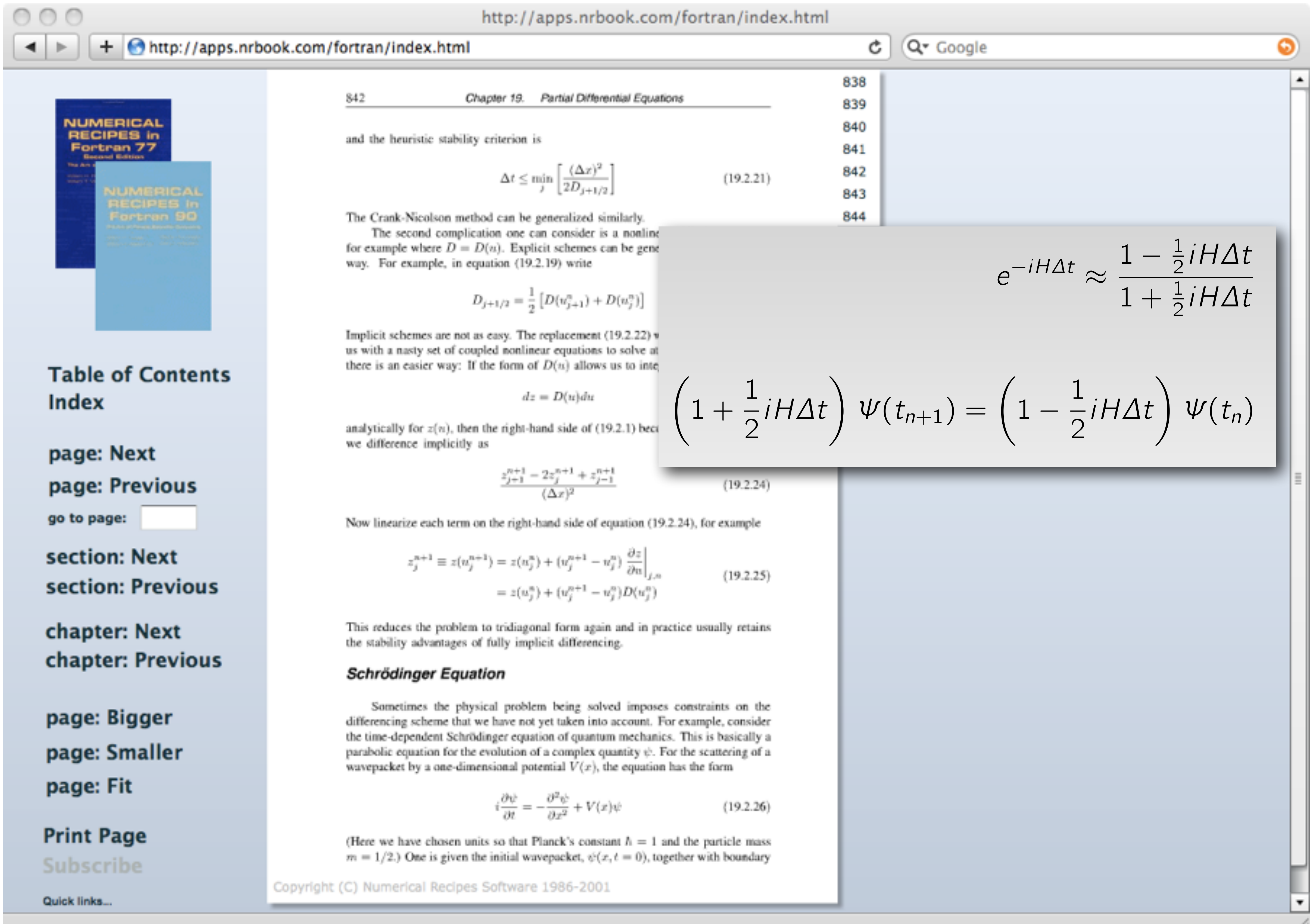
continuity equation for probability density

$$\frac{\partial |\Psi|^2}{\partial t} = -\vec{\nabla}\cdot\vec{j}$$

probability-density current

$$\vec{j} = -\frac{i\hbar}{2m}\left(\overline{\Psi}\,\vec{\nabla}\Psi - \Psi\,\vec{\nabla}\overline{\Psi}\right)$$

Crank-Nicolson algorithm



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and the heuristic stability criterion is

$$\Delta t \le \min_j \left[\frac{(\Delta x)^2}{2D_{j+1/2}} \right] \qquad (19.2.21)$$

The Crank-Nicolson method can be generalized similarly.

The second complication one can consider is a nonline
for example where $D = D(u)$. Explicit schemes can be gene
way. For example, in equation (19.2.19) write

$$D_{j+1/2} = \frac{1}{2}\left[D(u^n_{j+1}) + D(u^n_j)\right]$$

Implicit schemes are not as easy. The replacement (19.2.22) w
us with a nasty set of coupled nonlinear equations to solve at
there is an easier way: If the form of $D(u)$ allows us to inte

$$dz = D(u)du$$

analytically for $z(u)$, then the right-hand side of (19.2.1) bec
we difference implicitly as

$$\frac{z^{n+1}_{j+1} - 2z^{n+1}_j + z^{n+1}_{j-1}}{(\Delta x)^2} \qquad (19.2.24)$$

Now linearize each term on the right-hand side of equation (19.2.24), for example

$$\begin{aligned} z^{n+1}_j \equiv z(u^{n+1}_j) &= z(u^n_j) + (u^{n+1}_j - u^n_j)\left.\frac{\partial z}{\partial u}\right|_{j,n} \\ &= z(u^n_j) + (u^{n+1}_j - u^n_j)D(u^n_j) \end{aligned} \qquad (19.2.25)$$

This reduces the problem to tridiagonal form again and in practice usually retains the stability advantages of fully implicit differencing.

Schrödinger Equation

Sometimes the physical problem being solved imposes constraints on the differencing scheme that we have not yet taken into account. For example, consider the time-dependent Schrödinger equation of quantum mechanics. This is basically a parabolic equation for the evolution of a complex quantity ψ. For the scattering of a wavepacket by a one-dimensional potential $V(x)$, the equation has the form

$$i\frac{\partial \psi}{\partial t} = -\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi \qquad (19.2.26)$$

(Here we have chosen units so that Planck's constant $\hbar = 1$ and the particle mass $m = 1/2$.) One is given the initial wavepacket, $\psi(x, t = 0)$, together with boundary

$$e^{-iH\Delta t} \approx \frac{1 - \frac{1}{2}iH\Delta t}{1 + \frac{1}{2}iH\Delta t}$$

$$\left(1 + \frac{1}{2}iH\Delta t\right)\Psi(t_{n+1}) = \left(1 - \frac{1}{2}iH\Delta t\right)\Psi(t_n)$$

separation of variables

$$i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})\right)\Psi(\vec{r},t)$$

time-independent potential

ansatz: $\Psi(\vec{r},t) = A(t)\psi(\vec{r})$

$$i\hbar \frac{\partial A(t)}{\partial t}\psi(\vec{r}) = A(t)\,E\,\psi(\vec{r}) = A(t)\,\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})\right)\psi(\vec{r})$$

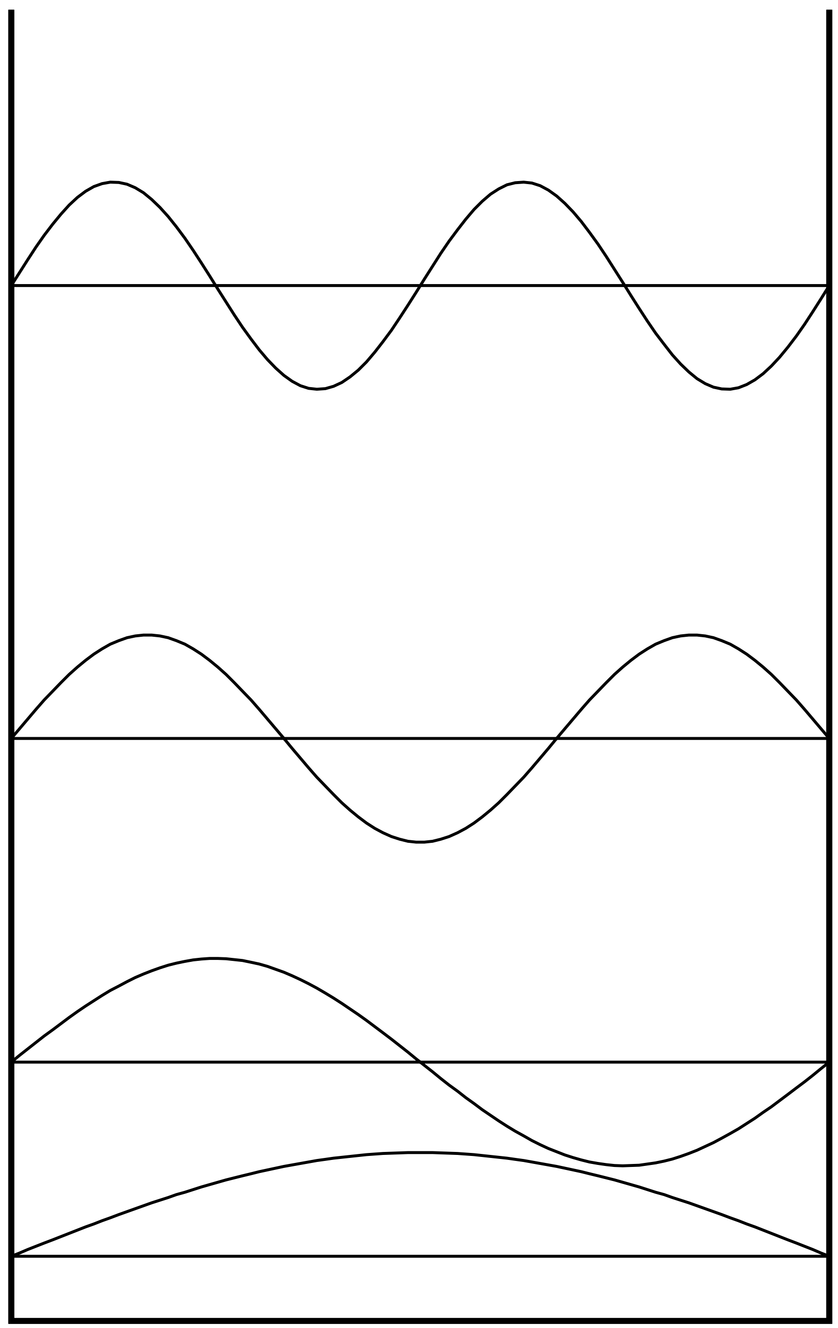
$$A(t) = A_0\, e^{-iEt/\hbar} \qquad \left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})\right)\psi(\vec{r}) = E\,\psi(\vec{r})$$

time-independent Schrödinger equation
(eigenvalue problem)

general solution: linear combination of eigenstates

$$\Psi(\vec{r},t) = \sum_n a_n\, e^{-iE_n t/\hbar}\,\psi_n(\vec{r})$$

particle in a box



boundary conditions ⇒ **quantization**

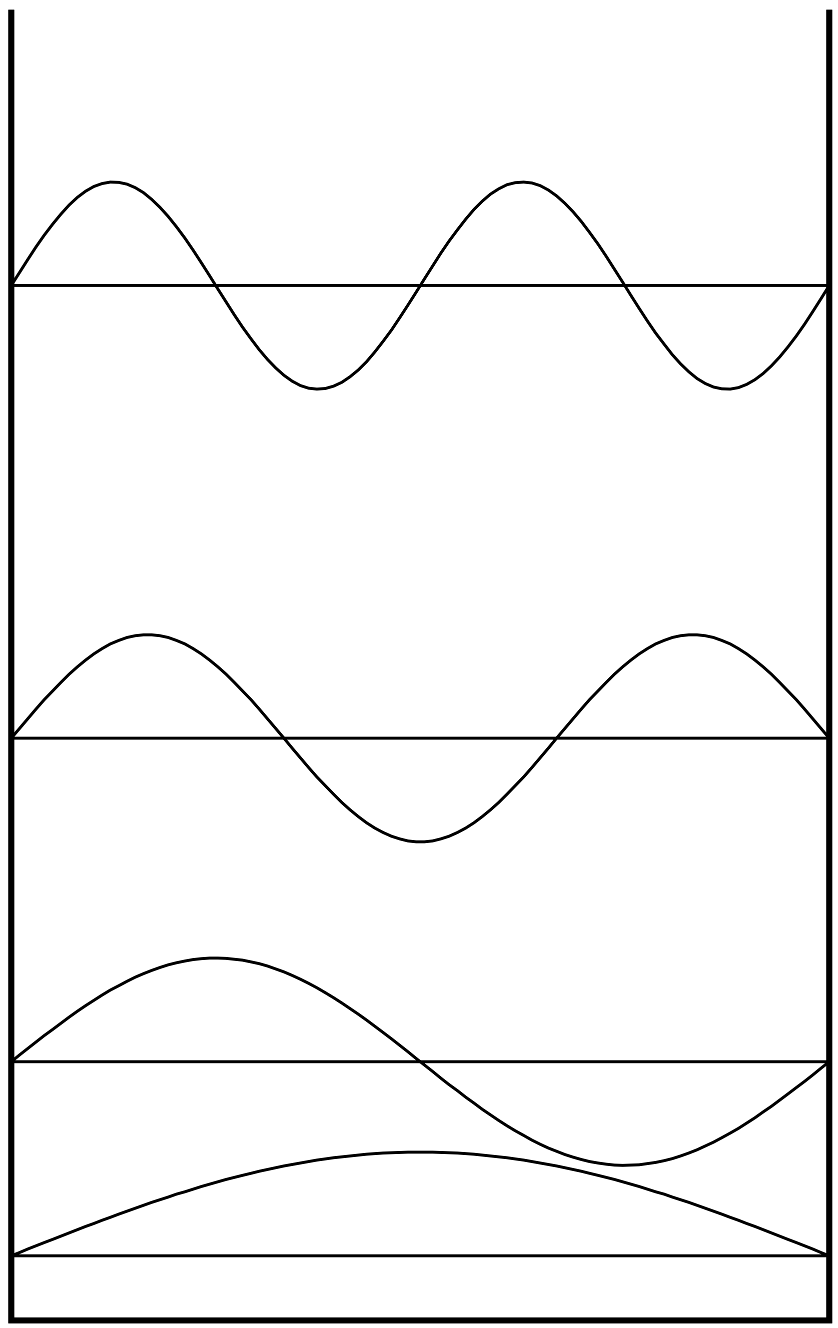
$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L_z}\right)^2$$

$$\varphi_n(z) = \sqrt{\frac{2}{L_z}}\sin\left(\frac{n\pi\, z}{L_z}\right)$$

discrete energies
zero-point energy
increasing number of nodes

symmetry of potential
symmetry of solutions (density)
even/odd eigenfunctions

particle in a box



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free wave packets

free time-independent Schrödinger equation: $$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x) = E\varphi(x)$$

eigenfunctions and -values: $$\varphi_k(x) = C\, e^{ikx}\,; \quad E_k = \frac{\hbar^2 k^2}{2m}$$

normalization: $$\int dx\, |\varphi_k(x)|^2 = C^2 \int_{-\infty}^{\infty} dx = ??$$

improper wave functions: $$\varphi_k(x) = \frac{1}{\sqrt{2\pi}}\, e^{ikx}$$

with ‘normalization’ as in Fourier transform:

$$\int dx\, \overline{\varphi_{k'}(x)}\, \varphi_k(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx\, e^{i(k-k')x} = \delta(k-k')$$

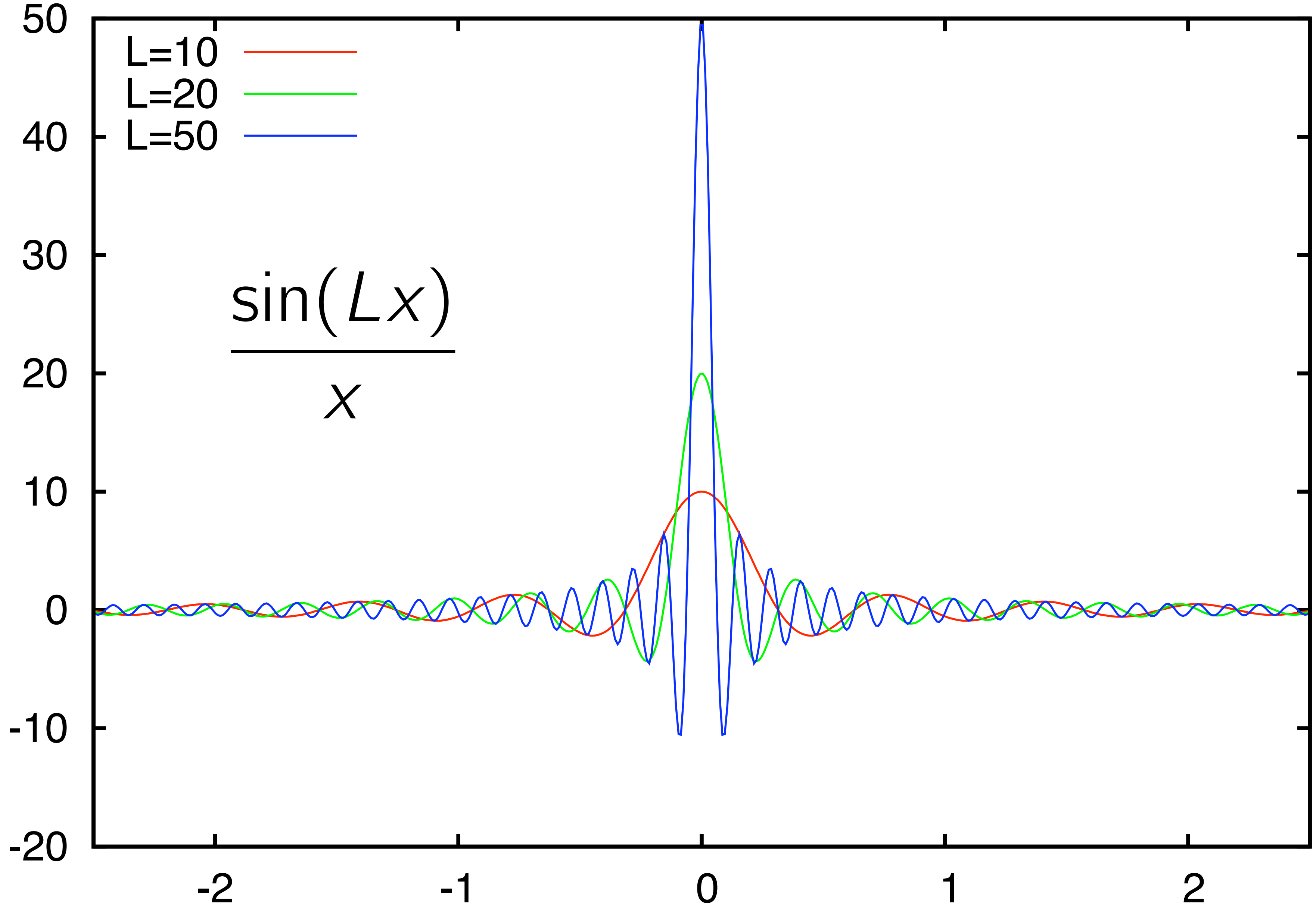
wave packet: normalizable linear combination of plane waves

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int dk\, \tilde{\varphi}(k)\, e^{i(kx-\omega(k)\,t)} \quad \text{with} \quad \int dk\, |\tilde{\varphi}(k)|^2 = 1$$

approximation to Dirac delta function

$$\int_{-L/2}^{L/2} dz\, e^{i(k_n-k_m)z} = \frac{1}{L}\,\frac{sin((k_n-k_m)\,L/2)}{(k_n-k_m)\,L/2} = \frac{1}{L}\,\delta_{n,m} \qquad (k_n = 2\pi n/L)$$

$$\int_{-\infty}^{\infty} dz\, e^{i(k-k')z} = \lim_{L\to\infty} \frac{2sin((k-k')\,L/2)}{(k-k')} = 2\pi\,\delta(k-k')$$



Gaussian wave packet

$$\tilde{\varphi}(k) = \frac{1}{\sqrt{\sqrt{2\pi}\,\sigma_k}}\, e^{-(k-k_0)^2/4\sigma_k^2}$$

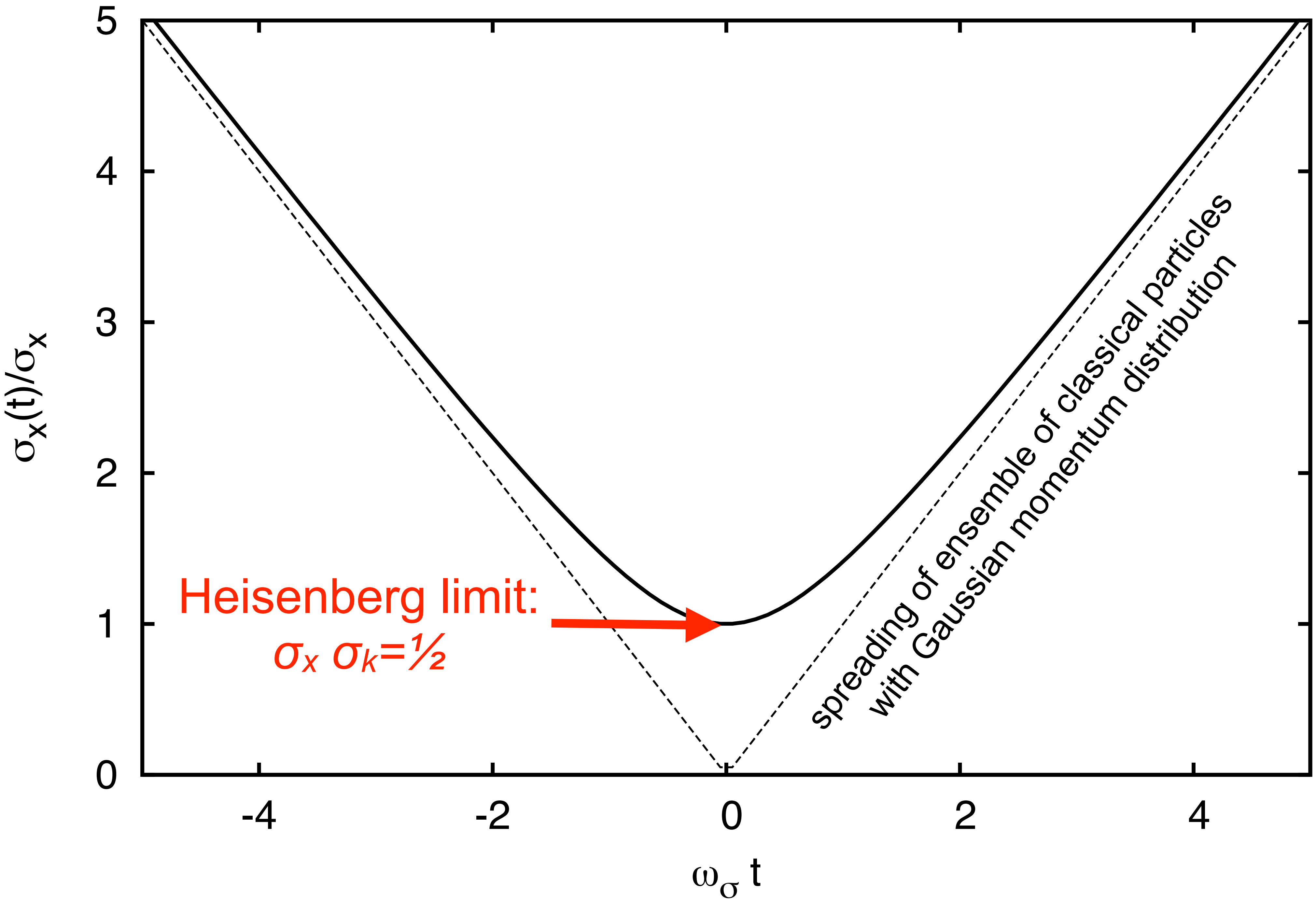
$|\tilde{\varphi}(k)|^2$ probability density for finding momentum $\hbar k$ is Gaussian of width σ_k, centered at k_0

$$\Psi(x,t) = \frac{1}{\sqrt{(2\pi)^{3/2}\sigma_k}} \int dk\, e^{-(k-k_0)^2/4\sigma_k^2}\, e^{i(kx-\omega(k)t)}$$

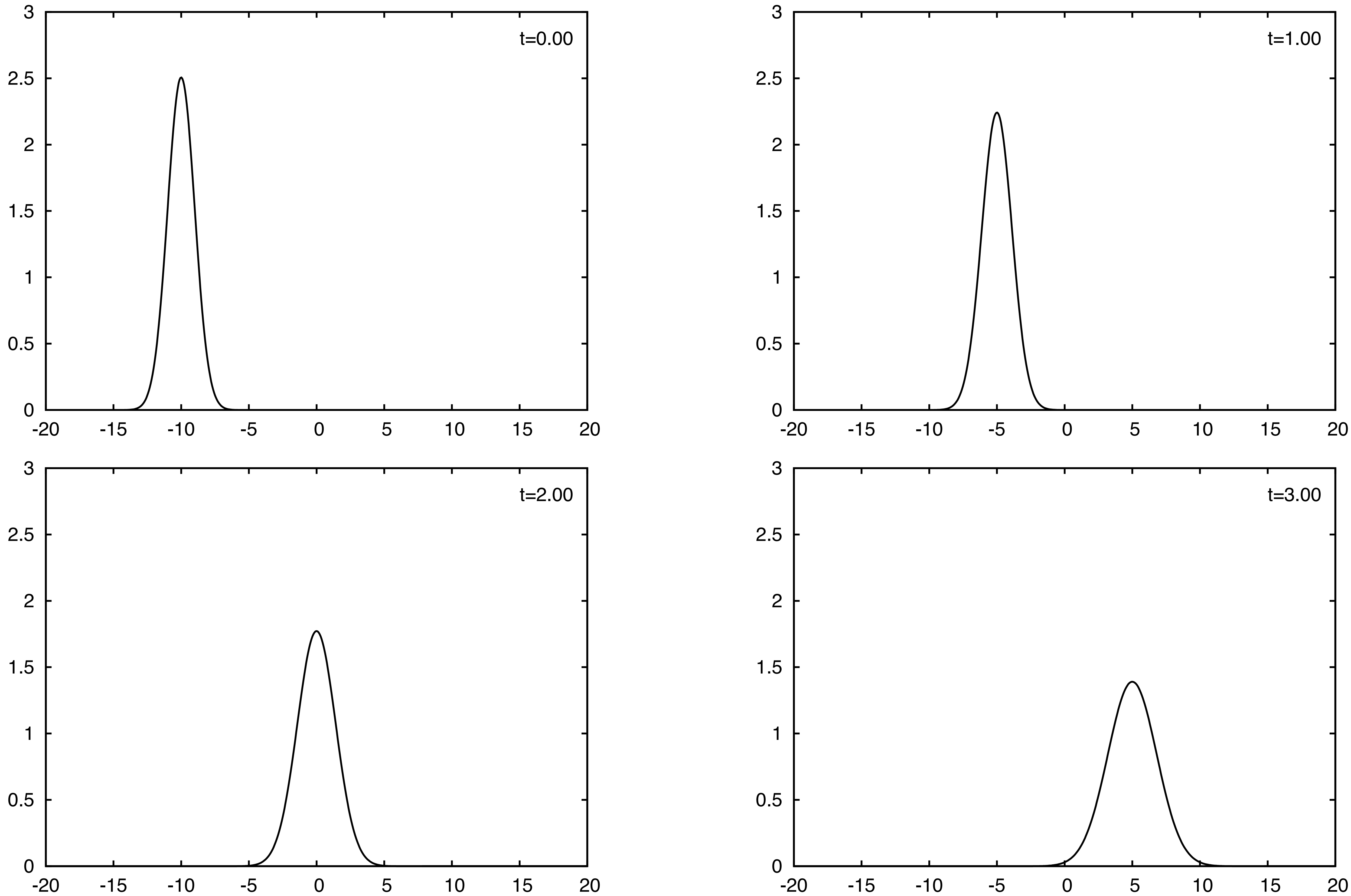
$$= \frac{1}{\sqrt{\sqrt{2\pi}\sigma_x(1+i\omega_\sigma t)}}\, e^{i(k_0 x-\omega(k_0)t)}\, e^{-\frac{(x-v_g t)^2}{4\sigma_x^2(1+i\omega_\sigma t)}}$$

probability density for finding particle at time t in position x is a Gaussian of width $\sigma_x\sqrt{1+\omega_\sigma^2 t^2}$, where $\sigma_x = 1/2\sigma_k$ and $\omega_\sigma = \hbar/2m\sigma_x^2$, with its center moving with the group velocity $v_g = \hbar k_0/m$.

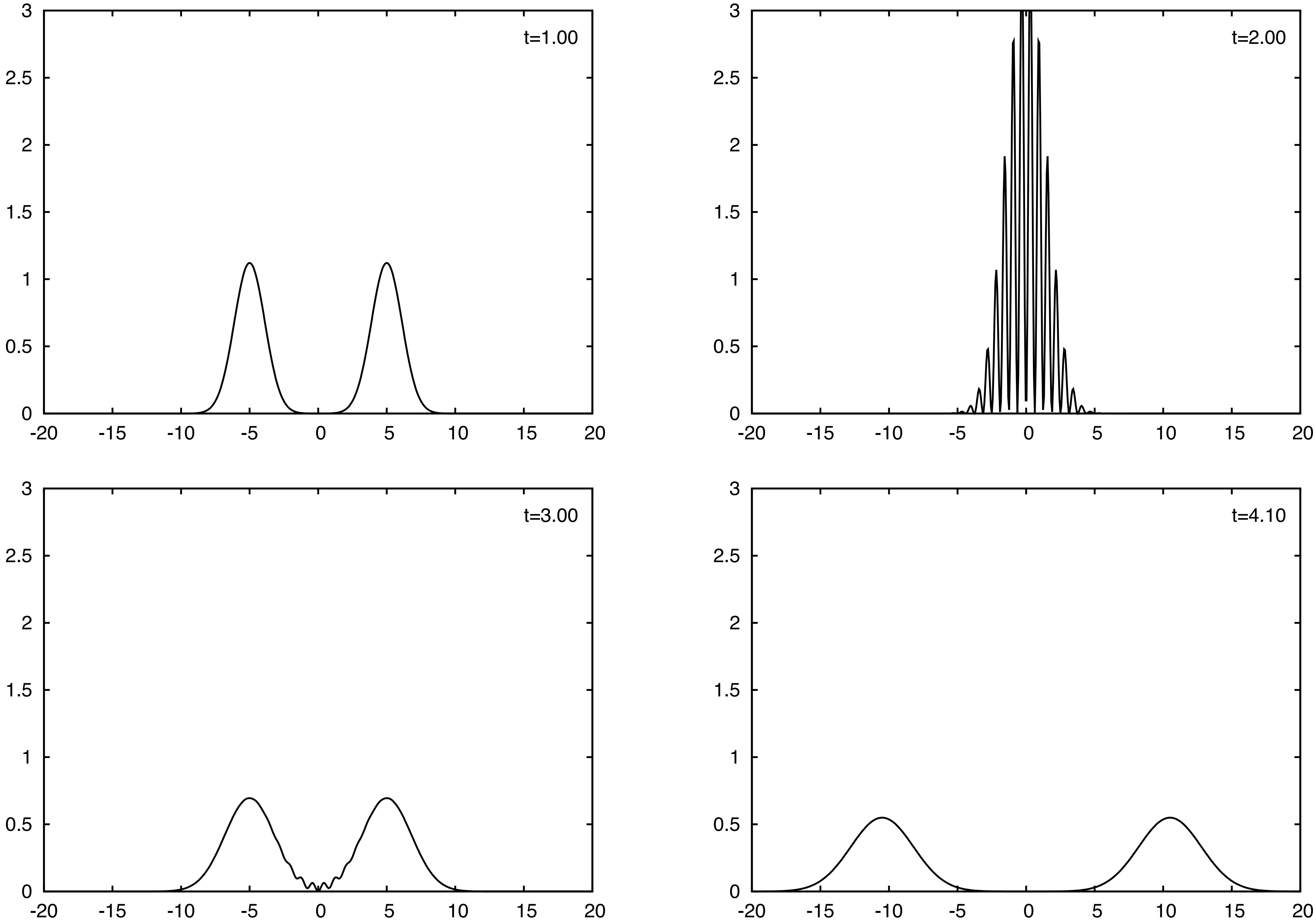
spreading of wave packet



wave packet



superposition of two wave packets



wave packet hitting infinite wall